A Pólya criterion for (strict) positive definiteness on the sphere

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Abstract

Positive definite functions are very important in both theory and applications of approximation theory, probability and statistics. In particular, identifying strictly positive definite kernels is of great interest as interpolation problems corresponding to these kernels are guaranteed to be poised. A Bochner type result of Schoenberg characterises continuous positive definite zonal functions, $f(\cos\cdot)$, on the sphere $\mathbb{S}^{d-1}$, as those with nonnegative Gegenbauer coefficients. More recent results characterise strictly positive definite functions on $\mathbb{S}^{d-1}$ by stronger conditions on the signs of the Gegenbauer coefficients. Unfortunately, given a function f, checking the signs of all the Gegenbauer coefficients can be an onerous, or impossible, task. Therefore, it is natural to seek simpler sufficient conditions which guarantee (strict) positive definiteness. We state a conjecture which leads to a Pólya type criterion for functions to be (strictly) positive definite on the sphere $\mathbb{S}^{d-1}$. In analogy to the case of the Euclidean space, the conjecture claims positivity of a certain integral involving Gegenbauer polynomials. We provide a proof of the conjecture for d from 3 to 8.

1 Introduction

Positive definite functions are very important in both theory and applications of approximation theory, probability and statistics. Although Bochner's theorem characterises continuous positive definite functions on $\mathbb{R}^d$ it has long been recognised that the conditions of Bochner's theorem may be difficult to check. For example Askey [4] states

> "It is an unfortunate fact that necessary and sufficient conditions are often impossible to verify and one must search for useful sufficient conditions when confronted with a particular example."

In 1918 Pólya [11] proved that an even, continuous function which is convex on the positive real line and vanishes at infinity has a non-negative Fourier transform. Later [12] he proved a similar statement for the inverse transform, thereby showing that an even function f which

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is continuous and convex on $[0, \infty)$, and vanishes at infinity, is positive definite on the real line. This sufficient condition is now commonly referred to as the *Pólya criterion*.

The criterion has been generalized for positive definite functions on $\mathbb{R}^d$ [3, 14, 17], considering radial functions instead of even ones. Further refinements of these criteria followed (cf. [10] and the references cited therein). Askey's proof [3] relates his Pólya type criterion to the non-negativity of certain integrals [7, 8]. These integrals represent the Fourier transform of a function, which can in some sense be considered as a prototype for all functions Askey's Pólya type criterion is applicable to.

A continuous function $g : [0, \pi] \to \mathbb{R}$ is (zonal) positive definite on the sphere $\mathbb{S}^{d-1}$ if for all distinct point sets $X = \{x_1, \ldots, x_n\}$ on the sphere and all $n \in \mathbb{N}$, the matrices $M_X := [g(d(x_i, x_j))]_{i,j=1}^n$ are positive semi-definite, that is, $c^T M_X c \geq 0$ for all $c \in \mathbb{R}^n$. In this definition $d(x, y)$ denotes the geodesic distance, $\arccos(x^T y)$, on $\mathbb{S}^{d-1}$. The function g is *strictly positive definite* on $\mathbb{S}^{d-1}$ if the matrices are all positive definite, that is, $c^T M_X c > 0$, for all nonzero $c \in \mathbb{R}^n$. The importance of strict positive definiteness is its connection with the poisedness of interpolation. Thus, if g is strictly positive definite on $\mathbb{S}^{d-1}$ then there is exactly one function of the form

$$s(x) = \sum_{j=1}^{n} \lambda_j g(d(x, x_j)),$$

which takes given values, $\{y_j\}_{j=1}^n$, at the distinct nodes $\mathcal{X} = \{x_j\}_{j=1}^n \subset \mathbb{S}^{d-1}$. Therefore, an easy means of identifying strictly positive definite kernels is of great interest as it will enable the assembly of a toolkit of different kernel based interpolation methods.

Continuous positive definite zonal functions on the sphere have been studied by Schoenberg [15] who proved the following theorem of Bochner type (Theorem 1 in [15]).

Theorem 1.1. *Let f be a continuous function on $[-1, 1]$. The function $f(\cos \cdot)$ is positive definite on $\mathbb{S}^{d-1}$ if and only if $f(\cos\theta)$ has a Gegenbauer expansion*

$$f(\cos\theta) \;=\; \sum_{k=0}^{\infty} a_k C_k^{\frac{d-2}{2}}(\cos\theta), \qquad \theta \in [0, \pi], \tag{1.1}$$

in which all of the coefficients a_k, $k \in \mathbb{N}_0$, are nonnegative, and $\sum_{k=0}^{\infty} a_k C_k^{\frac{d-2}{2}}(1) < \infty$.

The characterization of strictly positive definite functions on $\mathbb{S}^{d-1}$ came somewhat later. A simple sufficient condition [18] states that $f(\cos \cdot)$ is strictly positive definite if, in addition to the conditions of Theorem 1.1, all the Gegenbauer coefficients a_k are positive. Chen, Menegatto and Sun [5] showed that a necessary and sufficient condition for $f(\cos \cdot)$ be strictly positive definite on $\mathbb{S}^{d-1}$, $d \geq 3$, is that, in addition to the conditions of Theorem 1.1, infinitely many of the Gegenbauer coefficients with odd index, and infinitely many of those with even index, are positive.

Schoenberg also characterized those continuous functions $f : [-1, 1] \to \mathbb{R}$ such that $f(\cos \cdot)$ is a positive definite zonal function on all spheres (cf. (1.6) and Theorem 2 in [15]).

Theorem 1.2. *Let f be a continuous function on $[-1,1]$. The function $f(\cos\cdot)$ is positive definite on all spheres $\mathbb{S}^{d-1}$, $d \geq 2$, if and only if $f(\cos\theta)$ has an expansion*

$$f(\cos\theta) = \sum_{k=0}^{\infty} a_k (\cos\theta)^k, \qquad \theta \in [0,\pi], \tag{1.2}$$

where $a_k \geq 0$ for all $k \in \mathbb{N}_0$ and $\sum_{k=0}^{\infty} a_k$ converges.

A function $f : (c,d) \to \mathbb{R}$ is *absolutely monotonic*, if it has derivatives of all orders on (c,d), and these are all nonnegative. Such a function is characterized by having a series expansion

$$f(x) = \sum_{k=0}^{\infty} f^{(k)}(c^+)(x-c)^k, \tag{1.3}$$

converging to $f(x)$ for all $x \in (c,d)$. If in addition f is continuous on $[c,d]$ then the expansion converges to f uniformly on $[c,d]$. Therefore, Theorem 1.2 identifies the continuous functions $f : [-1,1] \to \mathbb{R}$ such that $f(\cos\cdot)$ is positive definite on all spheres, as those for which f is the analytic extension to $[-1,1]$ of an absolutely monotonic function on $[0,1]$.
Note that a similar result holds true for radial functions in $\mathbb{R}^d$, too, with absolute monotonicity being replaced by complete monotonicity. Theorem 1.2 hints towards what should be a Pólya type criterion for positive definite, zonal functions on the sphere. If we assume $f(\cos\cdot)$ to be positive definite on $\mathbb{S}^{d-1}$ only, we can expect the pattern (1.3) to break down after finitely many terms. This intuition fully applies in the Euclidean case $\mathbb{R}^d$.
The purpose of the present paper is to formulate a Pólya type criterion for positive definite, zonal functions on the sphere. The proof actually depends on proving non-negativity of a certain integral, see Conjecture 1.4 below. In parallel to the Euclidean theory, the proof in the general case turns out to be quite hard. We were able to establish the result for dimensions up to $d = 8$, doing extensive computer algebra and numerical calculations for higher dimensions.
Before stating the conjecture, let us first formulate the Pólya type criterion.

Theorem 1.3. *Let $d \in \{3,4,\ldots,8\}$ and $\lambda = \lceil \frac{d-2}{2} \rceil$. Let the real-valued function $g(\cdot) = f(\cos\cdot)$ on $[0,\pi]$ satisfy the following conditions:*

(i) $g \in C^{\lambda}[0,\pi]$,

(ii) *supp*$(g) \subset [0,\pi)$,

(iii) *the derivative, from the right, $g^{(\lambda+1)}(0)$ exists, and is finite,*

(iv) $(-1)^{\lambda} g^{(\lambda)}$ *is convex.*

Then g is a positive definite function on $\mathbb{S}^{d-1}$.

If, in addition to the above properties, $g^{(\lambda)}$, restricted to $(0,\pi)$, does not reduce to a linear polynomial, then g is a strictly positive definite function on $\mathbb{S}^{d-1}$.

We conjecture Theorem 1.3 to be true for all dimensions $d > 2$. Therefore, we will provide a proof for general dimension, relying on the following conjecture.

Conjecture 1.4. *Let $\delta > 0$, $\lambda > 0$ and $n \in \mathbb{N}_0$. For every $0 < t < \pi$, define*

$$F_n^{\lambda,\delta}(t) \;=\; \int_0^t (t-\theta)^\delta \, C_n^\lambda(\cos\theta)(\sin\theta)^{2\lambda}\, d\theta. \tag{1.4}$$

Then $F_n^{\lambda,\delta}(t) > 0$ for all t in $(0, \pi]$ if and only if $\delta \geq \lambda + 1$.

The conjecture is essentially equivalent to proving $(t-\theta)_+^\delta$ is strictly positive definite on $\mathbb{S}^{d-1}$. These zonal functions are supported on a spherical cap, as are the functions shown to be (strictly) positive definite in Theorem 1.3.

The conjecture has been stated in greater generality than we really need for the positive definiteness results for $\mathbb{S}^{d-1}$ of the form of Theorem 1.3. For those we are only interested in Gegenbauer coefficients for expansions with integer parameter, $\lambda = \lceil (d-2)/2 \rceil$.

The boundary case $\delta = \lambda + 1$ of Conjecture 1.4 will get special attention. Therefore, we define

$$F_n^\lambda(t) = F_n^{\lambda,\lambda+1}(t) = \int_0^t (t-\theta)^{\lambda+1} C_n^\lambda(\cos\theta)(\sin\theta)^{2\lambda}\, d\theta. \tag{1.5}$$

Those cases in which we have proven the conjecture are listed in the following proposition.

Proposition 1.5. *Let $d \in \{4, 6, 8\}$, $\lambda = (d-2)/2$ and $n \in \mathbb{N}_0$. Then*

$$F_n^\lambda(t) \;=\; \int_0^t (t-\theta)^{\lambda+1}\, C_n^\lambda(\cos\theta)(\sin\theta)^{2\lambda}\, d\theta > 0,$$

for all $0 < t \leq \pi$.

The observant reader will have noticed that the case $d = 2$, that is the case of the circle $\mathbb{S}^1$, does not appear in Theorem 1.3. This is because this particular case does not fit the general pattern for strict positive definiteness. Regarding positive definiteness Gneiting [9] has shown

Theorem 1.6. *Suppose the function $g(t)$, defined for $t \in [-K, K]$, has the following properties:*

(i) $g(t)$ *is real–valued, even, and continuous,*

(ii) $g(0) = 1$,

(iii) $\displaystyle\int_{-K}^{K} g(t)\, dt \geq 0$,

(iv) $g(t)$ *is nonincreasing and convex for* $t \in [0, K]$.

Then $g(t)$, $t \in [-K, K]$, is a correlation function on the circle circumference $2K$.

In the case $d = 2$, that is $\lambda = 0$, the function $F_n^0(t)$ is a multiple of $1 - \cos(nt)$. Therefore, it is not positive on all points $t \in (0, \pi]$, but rather has zeros at the points $t = 2k\pi/n$, $0 < k \leq \lfloor n/2 \rfloor$. Consequently, in order to guarantee all the Gegenbauer coefficients of g are strictly positive, as part of showing g is strictly positive definite, we have to assume slightly more than was required when $\lambda \in \mathbb{N}$. The methods used to show Theorem 1.3, with obvious modifications, yield the following:

Theorem 1.7. *Let the real-valued function $g(\cdot) = f(\cos \cdot)$ on $[0, \pi]$ satisfy the following conditions:*

(i) $g \in C[0, \pi]$,

(ii) $supp(g) \subset [0, \pi)$,

(iii) the derivative, from the right, $g'(0)$ exists, and is finite,

(iv) g is convex.

Then g is a positive definite function on $\mathbb{S}^1$.

If, in addition to the above properties, g, restricted to $(0, \pi)$, does not reduce to a piecewise linear function with finitely many pieces, then g is a strictly positive definite function on $\mathbb{S}^1$.

We omit the proof.

Notation: In the body of the paper many expressions will occur with removable singularities, consider for example (3.2) with $\lambda - \mu$ a negative integer. We interpret such expressions in the usual way, as the value of the limit.

2 A Polya criteria for $\mathbb{S}^{d-1}$

In this section we give a proof of Theorem 1.3 assuming the results regarding the positivity of the Gegenbauer coefficients of the functions $(t-\theta)_+^\mu$, $\mu = \lceil \lambda+1 \rceil$, listed in Proposition 1.5.

Recall that the Gegenbauer expansion of a function $g = f(\cos \cdot)$ is $g \sim \sum a_n C_n^\lambda$, where $a_n = b_n/h_n$,

$$b_n = b_n(g) = b_n^\lambda(g) = \int_{-1}^{1} f(x) C_n^\lambda(x) w_\lambda(x)\, dx = \int_0^\pi f(\cos\theta)\, C_n^\lambda(\cos\theta)\, (\sin\theta)^{d-2}\, d\theta, \quad (2.1)$$

and

$$h_n = h_n^\lambda = \int_{-1}^{1} \left\{C_n^\lambda(x)\right\}^2 w_\lambda(x)\, dx > 0. \quad (2.2)$$

We first give an alternative expression for the coefficients, $\{b_n\}$, which will provide a major part of a proof of the conjecture when the function g has two more continuous derivatives than is assumed in Theorem 1.3.

Lemma 2.1. *If $g \in C^{\lambda+2}[0,\pi)$ is identically zero in a neighbourhood of π then the coefficients, $\{b_n\}$, defined in (2.1), are alternatively given by the expression*

$$b_n(g) = \frac{(-1)^{\lambda+2}}{(\lambda+1)!} \int_0^\pi F_n^\lambda(\tau)\, g^{(\lambda+2)}(\tau)\, d\tau. \tag{2.3}$$

Proof: Applying Taylor's theorem with integral remainder

$$\begin{aligned} g(\theta) &= f(\cos\theta) \\ &= \sum_{k=0}^{\lambda+1} \frac{g^{(k)}(\pi)}{k!}(\theta-\pi)^k + \frac{1}{(\lambda+1)!}\int_\pi^\theta g^{(\lambda+2)}(\tau)(\theta-\tau)^{\lambda+1}\, d\tau \\ &= \sum_{k=0}^{\lambda+1} \frac{(-1)^k g^{(k)}(\pi)}{k!}(\pi-\theta)^k + \frac{(-1)^{\lambda+2}}{(\lambda+1)!}\int_\theta^\pi g^{(\lambda+2)}(\tau)(\tau-\theta)^{\lambda+1}\, d\tau, \quad \theta\in[0,\pi]. \end{aligned}$$

Therefore,

$$\begin{aligned} b_n = {}& \sum_{k=0}^{\lambda+1} \frac{(-1)^k g^{(k)}(\pi)}{k!} \int_0^\pi (\pi-\theta)^k\, C_n^\lambda(\cos\theta)\,(\sin\theta)^{2\lambda}\, d\theta \\ &+ \frac{(-1)^{\lambda+2}}{(\lambda+1)!}\int_0^\pi \int_\theta^\pi g^{(\lambda+2)}(\tau)(\tau-\theta)^{\lambda+1}\, d\tau\;\; C_n^\lambda(\cos\theta)\,(\sin\theta)^{2\lambda}\, d\theta \end{aligned}$$

Since all the derivatives at π vanish,

$$\begin{aligned} b_n &= \frac{(-1)^{\lambda+2}}{(\lambda+1)!}\int_0^\pi \int_0^\tau (\tau-\theta)^{\lambda+1}\, C_n^\lambda(\cos\theta)\,(\sin\theta)^{2\lambda}\, d\theta\;\; g^{(\lambda+2)}(\tau)\, d\tau \\ &= \frac{(-1)^{\lambda+2}}{(\lambda+1)!}\int_0^\pi F_n^\lambda(\tau)\, g^{(\lambda+2)}(\tau)\, d\tau. \qquad \square \end{aligned}$$

Proof of Theorem 1.3:
Restrict attention, for the moment, to the case of $d \in \{4,6,8\}$.
In order to apply the lemma we first have to mollify the function g.

Given $g \in C^\lambda[0,\pi)$, which is zero in a neigbourhood of π, we extend the definition of g to $[0,\infty)$ by taking $g(x)=0$ for all $x \geq \pi$. For $h>0$ define $G_h : [0,\infty) \to \mathbb{R}$ by

$$G_h(x) = \frac{1}{h^2}\int_0^h \int_0^h g(x+u+v)\, du\, dv. \tag{2.4}$$

Differentiating

$$G_h^{(\lambda)}(x) = \frac{1}{h^2}\int_0^h \int_0^h g^{(\lambda)}(x+u+v)\, du\, dv = \frac{1}{h^2}\int_x^{x+h}\int_0^h g^{(\lambda)}(w+u)\, du\, dw.s$$

Hence,

$$G_h^{(\lambda+1)}(x) = \frac{1}{h^2}\int_0^h \triangle_h\, g^{(\lambda)}(x+u)\, du, \tag{2.5}$$

where $\triangle_h$ is the usual forward difference operator. It follows that $G_h^{(\lambda+1)}$ is continuous on $[0,\infty)$. Further, rewriting (2.5) as

$$G_h^{(\lambda+1)}(x) = \frac{1}{h^2}\int_x^{x+h} \left[g^{(\lambda)}(w+h) - g^{(\lambda)}(w)\right]\, dw,$$

and differentiating,

$$G_h^{(\lambda+2)}(x) = \frac{1}{h^2}\triangle_h^2\, g^{(\lambda)}(x). \tag{2.6}$$

Hence $G_h^{(\lambda+2)}$ is also continuous on $[0,\infty)$.

Clearly G_h is supported in $[0,\pi)$ for all sufficiently small $h > 0$. Also, it follows from the uniform continuity of g, and (2.4), that $\{g_h\}$ converges uniformly to g on $[0,\pi]$, as $h \to 0^+$. Hence, fixing $n \in \mathbb{N}_0$ the coefficients $\{b_n(G_h)\}_{h>0}$ converge to $b_n = b_n(g)$, as $h \to 0^+$. By hypothesis $\psi := (-1)^\lambda g^{(\lambda)}$ is a convex function. Therefore, from (2.6), $(-1)^{\lambda+2}G_h^{(\lambda+2)}$ is a nonnegative function. Hence, since F_n^λ is nonnegative, it follows from Lemma 2.1 that the coefficient, $b_n = b_n(g)$, and therefore the Gegenbauer coefficient $a_n = b_n/h_n$, is nonnegative for all $n \in \mathbb{N}_0$.

We now turn to the question of the boundedness, or otherwise, of $\sum a_n C_n^\lambda(1)$.

We need some standard facts about convex functions, which can be found, for example, in [13]. The function ψ is convex on $[0,\pi)$. Therefore, it is absolutely continuous on every closed subset of $(0,\pi)$. The right and left derivatives of ψ exist at all points, $x \in (0,\pi)$, and are non-decreasing functions of x. These two one sided derivatives are continuous except at countably many points, and are equal at any point where one of them is continuous. Thus the two sided derivative of ψ exists, and is continuous, except at countably many points.

By hypothesis the one sided derivative $\psi'(0)$ also exists, and from the convexity it is a lower bound for the value of $\psi'(x)$ on $[0,\pi)$. Since $\psi'(\pi) = 0$, $\psi'(x) \le 0$ for all $x \in [0,\pi)$ for which it is defined. Using the absolute continuity of ψ, and defining $\eta_h = (-1)^\lambda G_h^{(\lambda)}$, (2.5) can be rewritten

$$\eta_h'(x) = \frac{1}{h^2}\int_0^h \int_0^h \psi'(x+v+u)\, dv\, du.$$

Thus $\eta_h'(x)$ is a weighted average of ψ' over the interval $(x, x+2h)$. Hence, for $0 \le x$,

$$\psi'(x) \le \eta_h'(x), \qquad \text{if } \psi'(x) \text{ exists}, \tag{2.7a}$$

and

$$\eta_h'(x) \le \psi'(x+2h), \qquad \text{if } \psi'(x+2h) \text{ exits}. \tag{2.7b}$$

Then, for $h > 0$,

$$\int_0^\pi \eta_h''(x)dx = \eta_h'(\pi) - \eta_h'(0) = 0 - \eta_h'(0) \le -\psi'(0) = (-1)^{\lambda+1}g^{(\lambda+1)}(0).$$

Using Lemma 2.1 it follows that

$$0 \leq b_n(G_h) \leq \frac{\|F_n^\lambda\|_\infty |g^{(\lambda+1)}(0)|}{(\lambda+1)!},$$

where $\|\cdot\|_\infty$ is the maximum norm on $[0,\pi]$. Taking the limit as $h \to 0^+$,

$$0 \leq b_n(g) \leq \frac{\|F_n\|_\infty |g^{(\lambda+1)}(0)|}{(\lambda+1)!}.$$

Lemma 3.6 shows that for $\lambda \in \mathbb{N}$, $\|F_n^\lambda\|_\infty = \mathcal{O}(n^{-3})$ as $n \to \infty$. Also, from [1, (22.2.3)],

$$h_n = \frac{\pi 2^{1-2\lambda}\Gamma(n+2\lambda)}{n!(n+\lambda)[\Gamma(\lambda)]^2} \approx n^{2\lambda-2} \qquad \text{and} \qquad C_n^\lambda(1) = \binom{n+2\lambda-1}{n} \approx n^{2\lambda-1}.$$

It follows from $a_n = b_n/h_n$, and the above, that $|a_n|C_n^\lambda(1) = \mathcal{O}(n^{-2})$. Hence the Gegenbauer series of g converges with $\sum |a_n(g)|C_n^\lambda(1) < \infty$. Combining the convergence of the series with the nonnegativity of the Gegenbauer coefficients, shown previously, the first part of Theorem 1.3 now follows as an application of Theorem 1.1.

We now turn to the part of the statement of Theorem 1.3 concerning strict postive definiteness.

We choose points $0 < 2a < b < \pi$ so that ψ, restricted to $[2a, b]$, is not a linear polynomial, and $\psi'(x)$ exists at $x = 2a$, and also at b. Therefore, $\psi'(2a) < \psi'(b)$. Choose $h_1 > 0$ so that $a < 2a - 2h_1 < b + 2h_1 < \pi$ and $0 < h < h_1$.
It follows from (2.7a) and (2.7b) that $\eta_h'(a-2h) \leq \psi'(2a)$ and $\psi'(b) \leq \eta_h'(b)$. Hence,

$$\int_a^b \eta_h''(x)\,dx \geq \int_{2a-2h}^b \eta_h''(x)\,dx = \eta_h'(b) - \eta_h'(2a-2h) \geq \psi'(b) - \psi'(2a) > 0.$$

Also $F_n^\lambda(\tau)$ is continuous and positive on the interval $[a,\pi]$. Thus, there is a number $\delta_n > 0$ such that $F_n^\lambda(\tau) \geq \delta_n$ for all τ in $[a,\pi]$. An application of Lemma 2.1 now shows that for each $n \in \mathbb{N}_0$, $b_n(G_h) \geq \delta_n \{\psi'(b) - \psi'(2a)\} > 0$. Since $0 < h < h_1$ was arbitary, taking the limit, as $h \to 0^+$, shows $b_n(g) > 0$. Hence all the Gegenbauer coefficients, $a_n = b_n/h_n$, of g are positive, and the sufficient condition of [18], discussed in the introduction, shows that g is strictly positive definite on $\mathbb{S}^{d-1}$.

The above has established both parts of Theorem 1.3 when $d \in \{4,6,8\}$. However, a function $g = f(\cos\cdot)$ which is (strictly) positive definite on $\mathbb{S}^{d-1}$ is necessarily (strictly) positive definite on $\mathbb{S}^{d-2}$. Hence, Theorem 1.3 for $d \in \{4,6,8\}$ implies Theorem 1.3 for $d \in \{3,5,7\}$.
□

We note that if the result of Proposition 1.5 were available for more values of $d \in 2\mathbb{N}$ then the above proof would immediately give Theorem 1.3 for more values of d.

Let us also note that increasing the power on $(t-\cdot)_+$ in the function $g(\cdot) = (t-\cdot)_+^\delta$ will preserve any existing positive definiteness. More precisely,

Lemma 2.2. *If $F_n^{\lambda,\delta}(t)$ is positive on $(0,\pi]$, except possibly for finitely many points t, then, for all $\mu > \delta$, $F_n^{\lambda,\mu}(t)$ is positive on $(0,\pi]$.*

Proof. This follows from the the semigroup property, $\mathcal{L}^{\delta+\mu} = \mathcal{L}^{\delta}\mathcal{L}^{\mu}$, for the fractional integrals

$$\mathcal{L}^{\delta} f := \frac{1}{\Gamma(\delta)} \int_0^t (t-\theta)^{\delta-1} f(\theta) d\theta. \quad \square$$

This lemma shows the pivotal role of the boundary case involving $F_n^{\lambda}(t)$.

3 Proofs of the conjecture in low dimensional cases

In this section we present proofs of the conjecture in low dimensional cases as detailed in Proposition 1.5.

Recall the formula connecting Gegenbauer polynomials with different parameters, [16, p. 99]. For $\mu > (\lambda-1)/2$,

$$(\sin\theta)^{2\mu}\, C_n^{\mu}(\cos\theta) = \sum_{k=0}^{\infty} c_{k,n}^{\mu,\lambda} (\sin\theta)^{2\lambda}\, C_{n+2k}^{\lambda}(\cos\theta), \tag{3.1}$$

where

$$c_{k,n}^{\mu,\lambda} = \frac{2^{2\lambda-2\mu}\Gamma(\lambda)\Gamma(n+2\mu)}{\Gamma(\mu)\Gamma(\lambda-\mu)} \frac{(n+2k+\lambda)(n+2k)!\,\Gamma(n+k+\lambda)\Gamma(k+\lambda-\mu)}{n!\,k!\,\Gamma(n+k+\mu+1)\Gamma(n+2k+2\lambda)}. \tag{3.2}$$

Note that if $\lambda-\mu$ is a negative integer the connection coefficient $c_{k,n}^{\lambda,\mu}$ is only nonzero for $0 \le k \le \mu-\lambda$.

Lemma 3.1. *For $\mu \ge 1$,*

$$C_n^{\mu}(\cos\theta)(\sin\theta)^{2\mu} = \sum_{k=0}^{\infty} c_{k,n}^{\mu} \cos(n+2k)\theta, \tag{3.3}$$

where

$$c_{k,n}^{\mu} := \frac{2^{1-2\mu}(-\mu)_k\Gamma(n+2\mu)\Gamma(n+k)(n+2k)}{\Gamma(\mu)n!\,k!\,\Gamma(n+k+\mu+1)}.$$

When $\mu \in \mathbb{N}$ the summation terminates at $k=\mu$ and the expression for $c_{k,n}^{\mu}$ can be rewritten as

$$c_{k,n}^{\mu} \;=\; \frac{2^{1-2\mu}}{\Gamma(\mu)}(-1)^k \binom{\mu}{k} \frac{(n+1)_{2\mu-1}(n+2k)}{(n+k)_{\mu+1}}. \tag{3.4}$$

Proof. Recall that $C_m^1(\cos\theta) = U_n(\cos\theta) = \sin(n+1)\theta/\sin\theta$. From the case $\lambda = 1$ of (3.1) we deduce that

$$\begin{aligned} C_n^\mu(\cos\theta)(\sin\theta)^{2\mu} &= \sum_{k=0}^{\infty} c_{k,n}^{\mu,1} \sin(n+2k+1)\theta\sin\theta \\ &= \frac{1}{2}\sum_{k=0}^{\infty} c_{k,n}^{\mu,1}(\cos(n+2k)\theta - \cos(n+2k+2)\theta \\ &= \frac{1}{2}\sum_{k=0}^{\infty}(c_{k,n}^{\mu,1} - c_{k-1,n}^{\mu,1})\cos(n+2k)\theta, \end{aligned}$$

so that $c_{k,n}^{\mu} = \frac{1}{2}c_{k,n}^{\mu,1} - \frac{1}{2}c_{k-1,n}^{\mu,1}$, the explicit formula of which is deduced from (3.2). $\square$

For μ a positive integer, equation (3.3) can also be deduced from the following relation for Gegenbauer polynomials,

$$(1-x^2)C_k^{\lambda+1}(x) = \frac{(k+2\lambda+1)(k+2\lambda)}{4\lambda(k+\lambda+1)}C_k^\lambda(x) - \frac{(k+2)(k+1)}{4\lambda(k+\lambda+1)}C_{k+2}^\lambda(x). \tag{3.5}$$

The equation (3.3) allows us to write down an explicit formula for $F_k^\lambda(t)$.

Lemma 3.2. *For* $\mu = 1, 2, 3, \ldots$,

$$\begin{aligned} F_n^{2\mu-1}(t) &= \sum_{k=0}^{2\mu-1} c_{k,n}^{2\mu-1}\frac{(-1)^\mu(2\mu)!}{(n+2k)^{2\mu+1}}\left[\sin(n+2k)t - \sum_{j=0}^{\mu-1}(-1)^j\frac{(n+2k)^{2j+1}}{(2j+1)!}t^{2j+1}\right], \\ F_n^{2\mu}(t) &= \sum_{k=0}^{2\mu} c_{k,n}^{2\mu}\frac{(-1)^{\mu+1}(2\mu+1)!}{(n+2k)^{2\mu+2}}\left[\cos(n+2k)t - \sum_{j=0}^{\mu}(-1)^j\frac{(n+2k)^{2j}}{(2j)!}t^{2j}\right]. \end{aligned}$$

Proof. It follows from Taylor's theorem with integral remainder that

$$\begin{aligned} \cos kt - \sum_{j=0}^{\mu}(-1)^j\frac{(kt)^{2j}}{(2j)!} &= (-1)^{\mu+1}\frac{k^{\lambda+2}}{(\lambda+1)!}\int_0^t (t-\theta)^{\lambda+1}\cos k\theta\, d\theta, \quad \lambda = 2\mu, \\ \sin kt - \sum_{j=0}^{\mu-1}(-1)^j\frac{(kt)^{2j+1}}{(2j+1)!} &= (-1)^{\mu}\frac{k^{\lambda+2}}{(\lambda+1)!}\int_0^t (t-\theta)^{\lambda+1}\cos k\theta\, d\theta, \quad \lambda = 2\mu-1. \end{aligned}$$

Consequently, together with the identity in Lemma 3.1, we obtain an explicit formula for $F_n^\lambda(t)$. $\square$

Prototypical special cases are,

$$\frac{4}{3}F_n^2(t) = \sum_{k=0}^{2}\frac{e_{k,n}}{(n+2k)^4}\left\{\cos((n+2k)t) - \left[1 - \frac{(n+2k)^2t^2}{2}\right]\right\}, \tag{3.6}$$

where

$$e_{0,n} = (n+3), \quad e_{1,n} = -2(n+2) \quad \text{and} \quad e_{2,n} = (n+1),$$

and

$$\frac{8}{3}\,F_n^3(t) = \sum_{k=0}^{3} \frac{f_{k,n}}{(n+2k)^5} \left\{ \sin((n+2k)t) - \left[(n+2k)t - \frac{(n+2k)^3\,t^3}{6} \right] \right\}, \tag{3.7}$$

where

$f_{0,n} = (n+5)(n+4)$, $f_{1,n} = -3(n+5)(n+2)$, $f_{2,n} = 3(n+4)(n+1)$ and $f_{3,n} = -(n+2)(n+1)$.

Let us write (3.5) as

$$\frac{2(k+\lambda+1)}{2\lambda+1}(1-x^2)\frac{C_k^{\lambda+1}(x)}{C_k^{\lambda+1}(1)} = \frac{C_k^{\lambda}(x)}{C_k^{\lambda}(1)} - \frac{C_{k+2}^{\lambda}(x)}{C_{k+2}^{\lambda}(1)}. \tag{3.8}$$

For $0 \le \delta \le \lambda$ define

$$G_n^{\lambda,\delta}(t) := \frac{F_n^{\lambda,\delta+1}(t)}{C_n^{\lambda}(1)} = \int_0^t (t-\theta)^{\delta+1} \frac{C_n^{\lambda}(\cos\theta)}{C_n^{\lambda}(1)}(\sin\theta)^{2\lambda}d\theta. \tag{3.9}$$

Then the following relation follows immediately from (3.8):

Lemma 3.3. *For $\lambda \in \mathbb{N}$ and $0 \le \delta \le \lambda$,*

$$\frac{2}{2\lambda-1}G_n^{\lambda,\delta}(t) = \frac{1}{n+\lambda}\left[G_n^{\lambda-1,\delta}(t) - G_{n+2}^{\lambda-1,\delta}(t)\right]. \tag{3.10}$$

Let us start from $\lambda = 0$ and make a change of variable in the integral to obtain

$$G_n^{0,\delta}(t) = \int_0^t (t-\theta)^{\delta+1}\cos n\theta d\theta = t^{\delta+2}\int_0^1 (1-s)^{\delta+1}\cos(nts)ds = t^{\delta+2}h_\delta(nt),$$

where

$$h_\delta(u) := \int_0^1 (1-s)^{\delta+1}\cos(us)ds. \tag{3.11}$$

Let us define

$$H_1^\delta(n,\xi_1,t) := h_\delta'((n+\xi_1)t) \tag{3.12}$$

and, for $j = 1, 2, \ldots$, define inductively

$$H_{j+1}^\delta(n,\xi_{j+1},\xi_j,\ldots,\xi_1,t) := \frac{\partial}{\partial\xi_{j+1}}\left[\frac{H_j^\delta(n+\xi_{j+1},\xi_j,\ldots,\xi_1,t)}{n+j+\xi_{j+1}}\right]. \tag{3.13}$$

Lemma 3.4. *For $j = 1, 2, \ldots,$,*

$$\frac{2^j}{(2j-1)!!}G_n^{j,\delta}(t) = (-1)^j\frac{t^{\delta+3}}{n+j}\int_{[0,2]^j} H_j^\delta(n,\xi_j,\ldots,\xi_1,t)d\xi_j\cdots d\xi_1. \tag{3.14}$$

Proof. Applying (3.10) with $\lambda = 1$ shows that

$$2G_n^{1,\delta}(t) = \frac{t^{\delta+2}}{n+1}\left[h_\delta(nt) - h_\delta((n+2)t)\right] = -\frac{t^{\delta+3}}{n+1}\int_0^2 h'_\delta((n+\xi)t)d\xi, \qquad (3.15)$$

which proves (3.14) when $j = 1$. For $j > 1$ we use induction and (3.10) to conclude

$$\frac{2^{j+1}}{(2j+1)!!}G_n^{j+1,\delta}(t) = \frac{(-1)^j t^{\delta+3}}{n+j+1} \times \int_{[0,2]^j}\left[\frac{H_j^\delta(n,\xi_j,\ldots,\xi_1,t)}{n+j} - \frac{H_j^\delta(n+2,\xi_j,\ldots,\xi_1,t)}{n+2+j}\right]d\xi_j\cdots d\xi_1,$$

from which the (3.14) for $j+1$ follows readily. □

In particular, for $j = 2$, this gives

$$\frac{4}{3}G_n^{2,\delta}(t) = \frac{t^{\delta+3}}{n+2}\int_0^2\int_0^2 \frac{\partial}{\partial\xi_2}\left[\frac{h'_\delta((n+\xi_1+\xi_2)t)}{n+1+\xi_2}\right]d\xi_2\,d\xi_1. \qquad (3.16)$$

Lemma 3.5. *For $r = 0, 1, 2, \ldots\lambda$,*

$$|h_\lambda^{(r)}(u)| \le c\,u^{-r-2}, \qquad \text{for } u \ge 1, \qquad (3.17)$$

where the constant c depends only on λ and r.

Proof. Let us denote by g_λ the function

$$g_\lambda(u) := (\lambda+1)!\begin{cases}(-1)^{\mu+1}\left[\cos u - \sum_{j=0}^{\mu}(-1)^j\frac{u^{2j}}{(2j)!}\right], & \lambda = 2\mu,\\ (-1)^{\mu}\left[\sin u - \sum_{j=0}^{\mu-1}(-1)^j\frac{u^{2j+1}}{(2j+1)!}\right], & \lambda = 2\mu-1.\end{cases}$$

From the displayed identities in the proof of Lemma 3.2, we then obtain $h_\lambda(u) = \dfrac{g_\lambda(u)}{u^{\lambda+2}}$. Since it is evident that $|g_\lambda(u)| \le c\ u^\lambda$ for $u \ge 1$, it follows that $|h_\lambda(u)| \le cu^{-2}$. Taking derivatives, it is easy to see that $|g_\lambda^{(j)}(u)| \le cu^{\lambda-j}$ for $1 \le j \le \lambda$ and $u \ge 1$. Consequently, by the Leibniz rule,

$$h_\lambda^{(r)}(u) = \sum_{j=0}^{r}\binom{r}{j}(-1)^j(\lambda+2)_j u^{-(\lambda+2+j)}g_\lambda^{(r-j)}(u),$$

from which the stated estimate follows. □

Lemma 3.6. *Let $\|\cdot\|_\infty$ denote the uniform norm on $[0,\pi]$. For $\lambda = 1, 2, \ldots,$*

$$\|F_n^\lambda\|_\infty = \mathcal{O}\left(n^{-3}\right), \quad \textit{as } n \to \infty.$$

Proof. Throughout this proof c represents a constant, possibly different at every occurrence, depending only on λ.

If $nt \leq 1$, then we use the expression of F_n^λ in Lemma 3.2, in which the terms in the square brackets are bounded by an absolute constant depending only on λ. Thus, the estimate $F_n^\lambda(t)| \leq cn^{-3}$ for $0 \leq t \leq n^{-1}$ follows immediately from the fact that the coefficients $c_{k,n}^\mu$ satisfies $|c_{k,n}^\mu| = \mathcal{O}(n^{\mu-1})$, see (3.4).

We now assume $0 < t \leq \pi$, $nt \geq 1$, and $\xi_i \in [0,2]$, for all i. Since $F_n^\lambda = C_n^\lambda(1) G_n^{\lambda,\lambda} = \binom{n+2\lambda-1}{n} G_n^{\lambda,\lambda}$, it is sufficient to show that $\max_{t\in[n^{-1},\pi]} |G_n^{\lambda,\lambda}(t)\| \leq c\, n^{-2\lambda-2}$. We claim that for $1 \leq j \leq \lambda$ the kernel H_j^λ of $G_n^{j,\lambda}$ in (3.14) is of the form

$$H_j^\lambda(n, \xi_j, \ldots, \xi_1, t) = \sum_{i=1}^{j} R_{i,j}(n, \xi_j, \ldots, \xi_1, t)\; h_\lambda^{(i)}((n + \xi_j + \ldots + \xi_1)t), \tag{3.18}$$

where the $R_{i,j}$ are rational functions of the form

$$R_{i,j} = \frac{P_{i,j}}{Q_{i,j}}, \qquad \deg(R_{i,j}) := \deg P_{i,j} - \deg Q_{i,j} \leq 1 + i - 2j, \tag{3.19}$$

where the $P_{i,j}$ are polynomials in $t, n, \xi_2, \ldots, \xi_j$; the $Q_{i,j}$ are polynomials in $n, \xi_2, \ldots \xi_j$; and their degrees refer to their highest degree in n. Furthermore,

$$\text{the coefficient of the highest power of } n \text{ in the polynomial } Q_{i,j} \text{ can be chosen as } 1. \tag{3.20}$$

Assume for now that (3.18), (3.19) and (3.20) have been shown. We then have

$$|R_{i,j}(n, \xi_j, \ldots, \xi_1, t)| = \mathcal{O}\left(n^{-(2j-i-1)}\right),$$

Since $nt \geq 1$ implies that $(n + \xi_j + \cdots + \xi_1)t \geq 1$, (3.17) and (3.18) then imply,

$$|H_j^\lambda(n, \xi_j, \ldots, \xi_1, t)| = \mathcal{O}\left(\sum_{i=1}^{j} n^{-(2j-i-1)}(nt)^{-i-2}\right) \leq c\, t^{-j-2} n^{-2j-1},$$

for $1 \leq j \leq \lambda$, where $0 \leq \xi_1, \ldots, \xi_j \leq 2$. Consequently, from (3.14) with $j = \lambda$ follows

$$\max_{t\in[n^{-1},\pi]} \left|G_n^{\lambda,\lambda}(t)\right| \leq \max_{t\in[n^{-1},\pi]} c\, t^{\lambda+3} t^{-\lambda-2} n^{-2\lambda-1} \leq c\, n^{-2\lambda-1},$$

which shows that $\max_{t\in[n^{-1},\pi]} \left|F_n^\lambda(t)\right| = \mathcal{O}\left(n^{-3}\right)$, and thus $\|F_n^\lambda\|_\infty = \mathcal{O}(n^{-3})$.

It only remains to prove (3.18), (3.19) and (3.20). The proof is by induction on j.

Induction basis: In the case $j = 1$ the identities follow from the definition (3.12), and the choice $P_{1,1} = Q_{1,1} = 1$.

Induction step: Assume that the properties have been established up to $j = k$. We shall leave out the argument of H_{k+1} and $R_{i,k+1}$ below and trust that no confusion is likely to occur. By (3.13) and the induction hypotheses,

$$H_{k+1}^\lambda = \sum_{i=1}^{k} \frac{\partial}{\partial \xi_{k+1}} \left[\frac{R_{i,k}(n + \xi_{k+1}, \xi_k, \ldots, \xi_1, t)}{n + k + \xi_{k+1}} h_\lambda^{(i)}((n + \xi_{k+1} + \ldots + \xi_1)t) \right],$$

from which we immediately deduce that (3.18) holds for H^{λ}_{k+1} with

$$R_{k+1,k+1} = t\frac{R_{k,k}(n+\xi_{k+1},\xi_k,\ldots,\xi_1,t)}{n+k+\xi_{k+1}}, \tag{3.21}$$

and, for $1 \le i \le k$, with $R_{0,k} := 0$,

$$\begin{aligned} R_{i,k+1} &= \frac{\partial}{\partial \xi_{k+1}}\left[\frac{R_{i,k}(n+\xi_{k+1},\xi_k,\ldots,\xi_1,t)}{n+j+\xi_{k+1}}\right] + t\frac{R_{i-1,k}(n+\xi_{k+1},\xi_k,\ldots,\xi_1,t)}{n+k+\xi_{k+1}} \\ &=: R^{(1)}_{i,k+1} + R^{(2)}_{i,k+1}. \end{aligned} \tag{3.22}$$

It follows from (3.21), by the induction hypotheses, that $\deg(R_{k+1,k+1}) = \deg(R_{k,k})-1 \le -k$. For $1 \le i \le k$, quick computations show that, by the induction hypotheses,

$$\deg(R^{(1)}_{i,k+1}) = \deg(R_{i,k}) - 2 \le i-1-2k, \quad \deg(R^{(2)}_{i,k+1}) = \deg(R_{i-1,k}) - 1 \le i-1-2k.$$

Finally, if $R = R_1 + R_2$ and $\max(\deg R_1, \deg R_2) = \ell$, then placing R_1 and R_2 over a common denominator, $\deg R \le \ell$. Consequently, by (3.22), $\deg R_{i,k+1} \le i-1-2k$. This shows (3.19) for $1 \le i \le k+1$ and $j = k+1$. Finally, (3.20) for $j = k+1$ and $1 \le i \le k+1$ follows from (3.21), (3.22) and the induction hythotheses. Thus, if the three properties hold up to $j = k$, they also hold for $j = k+1$.
Conclusion: The result follows by induction for all positive integers i and j, with $1 \le i \le j$. □

Proof of the case $d = 4$, that is $\lambda = 1$, of Proposition 1.5.

The case $n = 0$ is trivial. Assume now that $n > 0$. Recalling that $U_n(\cos(\theta)) = \sin((n+1)\theta)/\sin(\theta)$ we have

$$\begin{aligned} F^1_n(t) &= \int_{\theta=0}^{t} (t-\theta)^2\, U_n(\cos(\theta)) \sin^2\theta d\theta \\ &= \int_0^t (t-\theta)^2 \sin((n+1)\theta) \sin\theta\, d\theta \\ &= \frac{1}{2}\int_0^t (t-\theta)^2 \{\cos(n\theta) - \cos((n+2)\theta)\}\, d\theta \\ &= I(t,n) - I(t,n+2), \end{aligned} \tag{3.23}$$

where

$$I(t,m) = \frac{1}{2}\int_0^t (t-\theta)^2 \cos(m\theta)\, d\theta.$$

Integrating by parts shows that

$$I(t,m) = t^3 h(mt) \quad \text{with} \quad h(u) = \frac{u - \sin u}{u^3}, \quad u > 0. \tag{3.24}$$

Therefore

$$\frac{\partial}{\partial m} I(t,m) = -t^4 h'(mt) = -t^4 \, \frac{2u + u\cos u - 3\sin u}{u^4}, \tag{3.25}$$

where $u = mt$. By the trivial inequalities $|\cos u| \le 1$ and $|\sin u| \le 1$, we see that

$$g(u) := 2u + u\cos u - 3\sin u \ge 2u - u - 3 = u - 3 > 0, \qquad \text{for } u > 3.$$

On the other hand, the Taylor expansion of $g(u)$ takes the form

$$g(u) = 2\sum_{k=2}^{\infty} (-1)^k \frac{(k-1)u^{2k+1}}{(2k+1)!} = \frac{2u^5}{5!} - \frac{4u^7}{7!} + \frac{6u^9}{9!} - \frac{8u^{11}}{11!} + \dots$$

which is an alternating series, hence positive, if $0 < u^2 < 21$, which clearly covers $u \in (0,3]$. Consequently, it follows that $g(u) > 0$ for $u > 0$, which implies that for $t > 0$, $h(mt)$, hence $I(t,m)$, is strictly decreasing in $m > 0$. Therefore, by (3.23), $F_n^1(t)$ is positive for all $t > 0$ and all positive integers n. □

Proof of the case $d = 6$, that is $\lambda = 2$, of Proposition 1.5.

The proof below splits into two cases, t near zero, and $a/n < t \le \pi$, where a is a constant yet to be determined.

We deal with the second case first. Recall from (3.9) that $F_n^\lambda(t) = C_n^\lambda(1) G_n^{\lambda,\lambda}(t)$, and from (3.10),

$$\frac{2}{2\lambda - 1} G_n^{\lambda,\delta}(t) = \frac{1}{n+\lambda}\left[G_n^{\lambda-1,\delta}(t) - G_{n+2}^{\lambda-1,\delta}(t)\right].$$

We need to show that $G_n^{2,2}(t) > 0$, which holds if $\frac{d}{dn} G_n^{1,2}(t) < 0$.

From (3.15)

$$2\, G_n^{1,2}(t) = -\frac{t^5}{n+1}\int_0^2 h_2'((n+\xi)t)\,d\xi,$$

where h_2 is defined in (3.11). Therefore, writing h for h_2, we have

$$2t^{-5}\frac{d}{dn} G_n^{1,2}(t) = -\int_0^2 \left[\frac{t\,h''((n+\xi)t)}{n+1} - \frac{h'((n+\xi)t)}{(n+1)^2}\right] d\xi.$$

Our immediate goal is to find a constant a such that $\frac{d}{dn} G_n^{1,2}(t) < 0$ for $a/n < t \le \pi$, which will allow us to conclude that $F_n^2(t) > 0$, for $a/n < t \le \pi$. Evidently, it is sufficient to show that the function being integrated above is positive. Hence, we see that $\frac{d}{dn} G_n^{1,2}(t) < 0$ if

$$H(u) := (n+1)t\,h''((n+\xi)t) - h'((n+\xi)t) = \frac{n+1}{n+\xi} u h''(u) - h'(u) > 0, \tag{3.26}$$

for all $0 < \xi < 2$, where $u = (n+\xi)t$.

A simple calculation shows that

$$h(u) = h_2(u) = \frac{6}{u^4}\left(\cos(u) - 1 + \frac{u^2}{2}\right).$$

Next we show that for all $u > 0$, $h'(u) < 0$. Taking derivatives and Maclaurin series we see that

$$h'(u) = \frac{6\,(4 - u^2 - 4\cos u - u\sin u)}{u^5}$$
$$= \frac{6}{u^5}\sum_{k=3}^{\infty} \frac{2(-1)^k\,(k-2)}{(2k)!} u^{2k} = \frac{6}{u^5}\left(-\frac{u^6}{360} + \frac{u^8}{10080} - \frac{u^{10}}{604800} - \dots\right),$$

The series is an alternating series, and negative, for $u^2 < 28$, thus certainly for $0 < u \le 4$. Furthermore, when $u > 4$ the $-u^2$ dominates the other terms in the numerator and $h'(u)$ is again negative. The desired result follows.
Now we consider

$$h''(u) = \frac{6(-20 + 3u^2 - (-20 + u^2)\cos u + 8u\sin u)}{u^6}.$$

The trivial inequalities $|\sin u| \le 1$ and $|\cos u| \le 1$ show that

$$h''(u) \ge 6u^{-6}(3u^2 - u^2 - 8u - 40) = 12u^{-6}(u^2 - 4u - 20) > 0,$$

if $u > 2(1+\sqrt{6}) = 6.898989...$. In fact, numerical computation shows that $h''(u)$ has a single root for $0 < u < 7$ at $u_0 = 3.68542.....$ Thus, $h''(u)$ is positive if $u > u_0$. Combining these facts about h' and h'' we see that $H(u) > 0$ if $u > u_0$.
We now consider the case $0 < u \le u_0$ for which $h''(u) \le 0$. Then $0 < \xi < 2$ implies by (3.26)

$$H(u) \ge \frac{n+1}{n} u h''(u) - h'(u) \ge \frac{4}{3} u h''(u) - h'(u), \qquad \text{when } n \ge 3.$$

Define $k(u)$ to be the estimate of $H(u)$ from below given above

$$k(u) := \frac{4}{3} u h''(u) - h'(u) = \frac{u^{-5}}{3}\left[-92 + 15u^2 - 4(-20 + u^2)\cos u + 35u\sin u + 12\cos u\right].$$

Applying the trivial inequalities $|\cos u| \le 1$ and $|\sin u| \le 1$ shows that $k(u)$ is positive if $u > 5.9793....$ Numerical computation further shows that $k(u)$ has one single zero in $0 < u < 6$ at $u_1 = 1.86321....$ That is $k(u)$ is positive for all $u > u_1$.
Combining the results so far we have shown $H(u) > 0$ for all $u > u_1$. In view of the remarks near equation (3.26) this allows us to conclude that

$$F_n^2(t) > 0 \text{ whenever } u_1/n < t \le \pi, \text{ and } n \ge 3. \tag{3.27}$$

We still have to analyze the behaviour of $F_n(t)$ when $0 < t \le u_1/n$. By an inequality in [6], the largest zero of the Gegenbauer polynomial C_n^λ satisfies the inequality

$$x_{n,1}(\lambda) \le \frac{\sqrt{n^2 + 2(n-1)\lambda - 1}}{(n+\lambda)}.$$

Taking $t_n^* = \arccos(x_{n,1}(2))$ it follows that

$$\cos(t_n^*) = x_{n,1}(2) \le \sqrt{1 - \frac{9}{(n+2)^2}}$$

so that

$$(\sin t_n^*)^2 \ge \frac{9}{(n+2)^2},$$

and $C_n^2(\cos\theta)$ is positive whenever $0 < \theta < t_n^*$, and therefore whenever $0 < \theta \le \sin t_n^*$. By the definition of $F_n^2(t)$, this shows that

$$F_n^2(t) > 0 \quad \text{whenever } 0 < t \le 3/(n+2). \tag{3.28}$$

The regions of positivity given by equations (3.27) and (3.28) overlap when $n \ge 4$, so that for all such n, $F_n^2(t) > 0$ for all $0 < t \le \pi$. The same conclusion can be reached for $0 \le n \le 3$ by plotting the explicit expression (3.6) for $F_n^2(t)$. □

Proof of the case, $d = 8$ that is $\lambda = 3$, of Proposition 1.5.

The proof below splits into two cases, t near zero, and t greater than a/n, as did the proof in the $d = 6$ case.

We deal firstly with the case $t > a/n$. Recall from (3.9) that $F_n^\lambda(t) = C_n^\lambda(1)G_n^{\lambda,\lambda}(t)$, and from (3.10)

$$\frac{2}{2\lambda - 1} G_n^{\lambda,\delta}(t) = \frac{1}{n+\lambda}\left[G_n^{\lambda-1,\delta}(t) - G_{n+2}^{\lambda-1,\delta}(t)\right].$$

We need to show that $G_n^{3,3}(t) > 0$, which holds if $\frac{d}{dn} G_n^{2,3}(t) < 0$.
Our immediate goal therefore is to find a constant a so that $\frac{d}{dn} G_n^{2,3}(t) < 0$ for all $a/n < t \le \pi$.
By (3.16) with $\delta = 3$, and the function $h = h_3$, defined in (3.11),

$$\frac{4}{3} G_n^{2,3}(t) = \frac{t^6}{n+2} \int_0^2 \int_0^2 \left[\frac{th''((n+\xi+\eta)t)}{n+1+\eta} - \frac{h'((n+\xi+\eta)t)}{(n+1+\eta)^2}\right] d\eta\, d\xi.$$

Taking the derivative with respect to n and simplifying, we obtain

$$\begin{aligned}\frac{4}{3}\frac{d}{dn} G_n^{2,3}(t) = t^6 \int_0^2 \int_0^2 \Bigg[&\frac{t^2 h'''((n+\xi+\eta)t)}{(n+2)(n+1+\eta)} - \frac{(3n+5+\eta)th''((n+\xi+\eta)t)}{(n+2)^2(n+1+\eta)^2} \\ &+ \frac{(3n+5+\eta)h'((n+\xi+\eta)t)}{(n+2)^2(n+1+\eta)^3}\Bigg] d\eta\, d\xi.\end{aligned}$$

In order to show that $\frac{d}{dn} G_n^{2,3}(t) < 0$, we only need to show that the integrand is negative, for all $0 < \xi, \eta < 2$. We introduce a function

$$\begin{aligned} H_n(u) := u^2 h'''(u) &- \frac{(3n+5+\eta)(n+\xi+\eta)}{(n+2)(n+1+\eta)} uh''(u) \\ &+ \frac{(3n+5+\eta)(n+\xi+\eta)^2}{(n+2)(n+1+\eta)^2} h'(u). \end{aligned} \tag{3.29}$$

Then it is easy to see that

$$\frac{4}{3}\frac{d}{dn}G_n^{2,3}(t) = t^6 \int_0^2 \int_0^2 a_n H_n((n+\xi+\eta)t)\, d\eta\, d\xi, \tag{3.30}$$

where $a_n = a_n(\xi, \eta) = 1/((n+2)(n+1+\eta)(n+\xi+\eta)^2) > 0$. Thus, to demonstrate that $\frac{d}{dn}G_n^{2,3}(t)$ is negative, it is sufficient to show that $H_n(u) < 0$ for all $0 < \xi, \eta < 2$, where $u = (n+\xi+\eta)$.
Now, a simple computation shows that

$$h(u) = h_3(u) = \int_0^1 (1-s)^4 \cos(su) ds = \frac{4(-6u + u^3 + 6\sin u)}{u^5}.$$

Therefore

$$\begin{aligned}
h'(u) &= -\frac{8(u^3 - 12u - 3u\cos u + 15\sin u)}{u^6}, \\
h''(u) &= \frac{24(u(u^2-20) - 10u\cos u - (u^2-30)\sin u)}{u^7}, \\
h'''(u) &= -\frac{24(4u(u^2-30) + u(u^2-90)\cos u - 15(u^2-14)\sin u)}{u^8}.
\end{aligned}$$

It is immediately clear that for all large u the signs of the $h^{(j)}(u)$ alternate in such a way as to make $H_n(u)$ (defined in (3.29)) negative. We need a good estimate of just how large u must be.

The signs $h^{(j)}(u)$ can be determined as in the previous cases. It turns out that $h'(u) < 0$ for all $u > 0$. Elementary consideration shows that $h''(u) > 0$ for all large u and numerical computation shows that $h''(u)$ has one simple zero for $u > 0$ at $u_2 = 4.23573...$, so that $h''(u) > 0$ for $u > u_2$ and $h''(u) < 0$ for $0 < u < u_2$. Similarly, $h'''(u)$ has one simple zero for $u > 0$ at $u_3 = 7.15125...$, $h_3'''(u) < 0$ for $u > u_3$ and $h'''(u) > 0$ for $0 < u < u_3$. We have several cases.

Case 1. $u \geq u_3$. In this case, $h'(u) < 0$, $h''(u) > 0$ and $h'''(u) \leq 0$. That $H_n(u) < 0$ then follows immediately from the definition in (3.29).

Case 2. $0 < u < u_3$. We write $H_n(u)$ as

$$H_n(u) = u^2 h'''(u) - \frac{(3n+5+\eta)(n+\xi+\eta)}{(n+2)(n+1+\eta)}\left[uh''(u) - \frac{n+\xi+\eta}{n+1+\eta}\, h'(u)\right].$$

Since $h'(u) < 0$ it follows readily that for $0 < \xi, \eta < 2$,

$$\begin{aligned}
uh''(u) - \frac{n+\xi+\eta}{n+1+\eta}\, h'(u) &> uh''(u) - \left(1 - \frac{1}{n+1+\eta}\right) h'(u) \\
&> uh''(u) - \left(1 - \frac{1}{n+1}\right) h'(u) \geq uh''(u) - h'(u)/2 > 0,
\end{aligned}$$

if $u > u_0 = 2.99521...$, and the last quantity on the right of the display is zero at $u = u_0$. Consequently, we obtain that for $u > u_0$,

$$H_n(u) < u^2 h'''(u) - \left(3 - \frac{1}{n+2}\right)\left(1 - \frac{1}{n+1}\right)\left[u h''(u) - \left(1 - \frac{1}{n+1}\right) h'(u)\right].$$

Denote the right hand side of the above inequality by $\Lambda_n(u)$. $\Lambda_n(u)$ is positive at u_0 if $n = 1$ and is negative at u_3 for all $n \in \mathbb{N}$. It is also a decreasing function of n for $u_0 < u$. Numerical computation shows that

$$\Lambda_9(u) < 0, \qquad \text{if} \quad u > u^* = 3.63661....$$

This shows that $H_n(u) < 0$ for $u^* < u \leq u_3$ and $n \geq 9$.

We have already shown in case 1 that $H_n(u) < 0$ if $u \geq u_3$. Hence $H_n(u) < 0$ on (u^*, ∞), if $n \geq 9$. As $u = (n + \xi + \eta)t$, it follows by (3.30) that $\frac{d}{dn} G_n^{2,3}(t) > 0$ if $nt > u^*$ or $t > u^*/n$. Consequently, by (3.10) and (3.9) we conclude that $F_n^3(t) = C_n^3(1)\, G_n^{3,3}(t) > 0$ if $t > u^*/n$ and $n \geq 9$.
On the other hand, an inequality in [2] shows that the largest zero of the Gegenbauer polynomial C_n^λ satisfies the inequality

$$x_{n,1}(\lambda) \leq \sqrt{\frac{(n-1)(n+2\lambda-2)}{(n+\lambda-2)(n+\lambda-1)}} \cos \frac{\pi}{n+1}.$$

Therefore, defining $t_n^* = \arccos(x_{n,1}(3))$,

$$\cos^2 t_n^* \leq \frac{(n-1)(n+4)}{(n+1)(n+2)} \cos^2 \frac{\pi}{n+1},$$

and

$$\sin t_n^* \geq \sqrt{1 - \left(1 - \frac{6}{(n+1)(n+2)}\right) \cos^2 \frac{\pi}{n+1}}. \tag{3.31}$$

$C_n^3(\cos\theta)$ is positive for $0 < \theta < t_n^*$, and therefore, from its definition, $F_n^3(t)$ is positive for $0 < t \leq \sin(t_n^*)$. Estimating $\sin t_n^*$ from below we have

$$\sin t_n^* \geq \sqrt{1 - \left(1 - \frac{6}{(n+1)^2}\right)\left(1 - \frac{\pi^2}{2(n+1)^2} + \frac{\pi^4}{24(n+1)^4}\right)^2} = \frac{\sqrt{6+\pi^2}}{n+1} + \mathcal{O}\left(\frac{1}{n^2}\right). \tag{3.32}$$

At this point we have shown $F_n^3(t)$ to be positive on $(0, \sin(t_n^*)]$ and also on $(u^*/n, \pi]$. Since $\sqrt{6+\pi^2} = 3.983667.. > u^*$ the asymptotic estimate of $\sin(t_n^*)$ above shows that the regions on which $F_n^3(t)$ is positive overlap, and cover all of $(0, \pi]$, for all large enough n. Numerical comparison of $\sin t_n^*$ and u^*/n shows that the overlap happens for all $n > 14$. The proof of the positivity of $F_n^3(t)$ on $(0, \pi]$, when $0 \leq n \leq 14$, can be completed by plotting the explicit expression (3.7) for $F_n^3(t)$ on $[0, \pi]$. $\square$

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